§7. Microwave Heating of Liquid Water and Ice: Molecular Dynamics Study

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By molecular dynamics simulations we have shown that water is heated by applied microwave through excitation of rotational alignment and subsequent relaxation of electrical dipoles. Crystal ice is much less heated due to hydrogen-bonded molecular network.

Electromagnetic waves heat solid, liquid and gaseous matters such as engineering materials, laboratory plasmas and biological matters including living cells. A microwave ovens used in daily food processing is one of such examples. The purpose of this study is to investigate the heating process of water and salt solutions by applied microwaves in terms of classical molecular dynamics simulation.

We use the microwaves of 10GHz whose wavelength is 3cm. Since the molecular scale is much less than this length, and since all the involved velocities are much less than the speed of light ($v/c<<1$), we can safely assume that the waves are spatially uniform, time varying electric field of the form $E(t)= E_0\cos(\omega t)$. Water molecules are represented by the rotating rigid body known as the SPC water model [1]. We adopt crystal ice for the initial conditions with randomized O-H directions [2]. These molecules move under the Coulomb and Lennard-Jones forces which are exerted by surrounding molecules [3].

Fig.1 shows the time history of the applied microwave field, the potential energy (Coulombic + Lennard-Jones), and the total energy of the system. The observed heating is attributed to the increase in the translational energy resulting from rotation excitation and relaxation of water molecules. Distributions of the water dipoles in terms of the directional cosine of their angles with the x-axis $\cos\Theta$ are shown in Fig.2. For room temperature water, the molecular dipoles distribute randomly. However, with the finite microwave field the dipoles align along the electric field direction and follow at each instant the statistical (Boltzmann) distribution $\exp(-Ed\cos\Theta /kT)$ [d is the dipole moment of H_2O].

By contrast, the water in ice state is hardly heated by microwave. This is due to the formation of hydrogen-bonded network in crystal ice. The bird's-eye view of H_2O molecules for the ice state in Fig.3 reveals this situation.

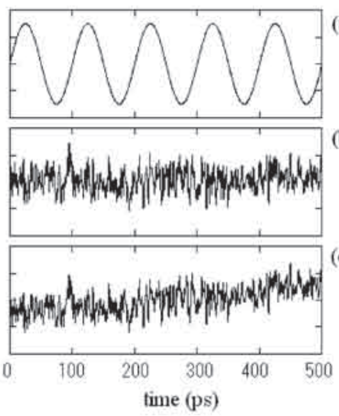

Fig.1: The time history of (a) the applied microwave field, (b) potential energy and (c) total energy of the system for water.

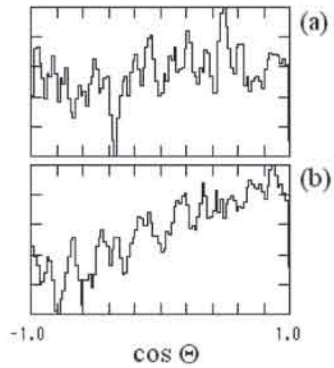

Fig.2. The distribution of water dipoles (logarithmic scale) in terms of the angles Θ with the x-axis for water of 300K. The microwave electric field is null in (a) and points to the x direction in (b).

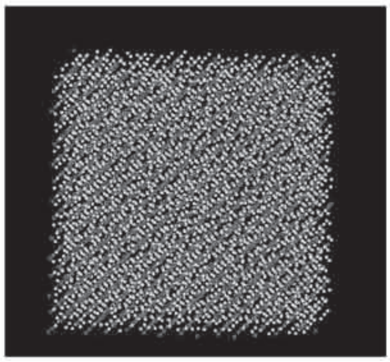

Fig.3 Bird's-eye view of 2700 H_2O molecules in ice state.

References

[1] H.Berendsen, J.Grigera, T.Straatsma, J.Phys. Chem. 91, 6269 (1987)
[2] Courtesy of Dr. M.Matsumoto
[3] Y.Rabin and M.Tanaka, Phys.Rev.Lett., 94, 148103 (2005)